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A NUMERICAL SCHEME TO SOLVE

div $\underline{u} = \rho$, curl $\underline{u} = \zeta$

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A NUMERICAL SCHEME TO SOLVE

div $\underline{u} = \rho$, curl $\underline{u} = \underline{\zeta}$

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Abstract

A compact finite difference scheme and a related box-scheme are described for solving div $\underline{u} = \rho$, curl $\underline{u} = \underline{\zeta}$ without the use of vector and scalar potentials.

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Introduction

This paper describes a finite difference scheme for the numerical solution of $\operatorname{div} \underline{u} = \rho$, $\operatorname{curl} \underline{u} = \underline{\zeta}$ in $\mathbb{R}^3$ which does not employ vector and scalar potentials.

A difficulty in considering any naive finite difference scheme for these equations arises from the fact that the differential equations are overdetermined unless the compatability condition $\operatorname{div} \operatorname{curl} \underline{u} = 0$ is imposed and there is then a need to describe a determined system of algebraic equations for $\underline{u}$. This problem does not arise in two dimensions where a scheme for the Cauchy-Riemann equations, similar to that proposed here, was described in Rose [4] and was effectively employed by Gatski, Grosch, and Rose [1]. However, the discussion in [4] lacked a satisfactory proof of convergence.

A fact of theoretical and practical importance is that the solution of the differential equations may be obtained in the form $\underline{u} = \underline{v} + \underline{w}$ where $\operatorname{div} \underline{v} = 0$ and $\operatorname{curl} \underline{w} = 0$. We shall show that a related decomposition applies to the finite problem as well. However, we shall not introduce the vector and scalar potentials $\underline{v} = \operatorname{curl} \underline{z}$, $\underline{w} = \operatorname{grad} \phi$ by means of which the continuous problem may, by employing a particular solution of $\operatorname{curl} \operatorname{curl} \underline{z} = \underline{\zeta}$, be reduced to solving $\nabla^2 \phi = \rho$. By not employing such potentials we hope to examine the algebraic problem underlying a direct finite difference approach to the system of differential equations and, also, to describe a scheme which may be of practical use when, as is common, accurate values of $\operatorname{grad} \underline{u}$ at the boundary of a domain are required and which need not be simply accomplished when finite difference schemes based upon potential formulations are employed.

Noting that the most useful identities which lead to norm estimates for the solution of the continuous problem are based upon the use of integration-by-parts we introduce at the outset an inner product in a finite approximation space and then impose conditions which permit summation-by-parts to play the same role in the finite problem as integration-by-parts plays in the continuous case. This leads directly to a variational formulation of the finite problem and the resulting finite difference equations (given by (3.1) and (3.2)) emerge as the admissibility conditions and the Euler equations for the variational problem. A natural consequence, also, are norm estimates whose use immediately establishes the convergence of the scheme. While these estimates imply that the central differences of the solution $\underline{u}_h$ of the finite difference scheme as well as $\underline{u}_h$ itself are first order accurate these results may not the best possible since, in the two-dimensional case, numerical results indicate that $\underline{u}_h$ is second order accurate [1].

The finite difference equations (3.1) and (3.2) which arise from this approach are compact in the sense that they describe relationships between values of $\underline{u}_h$ on the faces of a representative computational cell. They also lead, with a considerable reduction in computational effort, to a box-scheme in which variables associated with the vertices of a cell are employed. While an SOR type of solution method due to Kaczmarz [3] can be employed to solve this type of system, methods more specific to equations of this type would be highly desirable. We plan to report on several such methods in a forthcoming paper.

1. A Summation Identity

Let D be a bounded region in $\mathbb{R}^3$ with boundary Γ on which $\underline{n}$ is the outward unit normal. We consider a steady, inviscid, incompressible flow in D having specified distributions of vorticity $\underline{\zeta}$ and sources ρ, the mass flux over the surface being prescribed. Thus, if $\underline{u}$ is the velocity, then

$$\text{(1.1)} \qquad \begin{aligned} \operatorname{curl} \underline{u} &= \underline{\zeta}\,, \ \operatorname{div} \underline{u} = \rho && \text{in } D \\ \underline{u}\cdot\underline{n} &= g && \text{on } \Gamma, \end{aligned}$$

where, necessarily,

$$\int_\Gamma g\,dA = \int_D \rho\,dv, \quad \int_\Gamma (\underline{\zeta}\cdot\underline{n})\,dA = 0,$$

in which the latter condition arises from $\operatorname{div} \operatorname{curl} \underline{u} = 0$.

An easily established identity resulting from the use of integration by parts is

$$\text{(1.2)} \qquad \|\operatorname{grad} \underline{u}\|^2 = \int_D \left[(\operatorname{div} \underline{u})^2 + (\operatorname{curl} \underline{u})^2\right] dv + \int_\Gamma (\underline{u}\cdot\nabla)(\underline{u}\cdot\underline{n})\,dA,$$

in which

$$\operatorname{grad} \underline{u} \equiv (\partial_{x_1}, \partial_{x_2}, \partial_{x_3})\underline{u}$$

$\left(\partial_{x_i} \equiv \dfrac{\partial}{\partial x_i}\right)$ and

$$\|\operatorname{grad} \underline{u}\|^2 \equiv \int_D (\operatorname{grad}^2 u_1 + \operatorname{grad}^2 u_2 + \operatorname{grad}^2 u_3)\,dV.$$

Cover D by regular cells $\{\pi\}$ each of volume $\Delta V = \Delta x_1 \Delta x_2 \Delta x_3$ whose faces are parallel to the coordinate axes; the result is a covering domain D_h, $h = \max_i \Delta x_i$, whose corresponding boundary Γ_h is formed by faces of $\{\pi\}$ each of representative area ΔA. Define

$$
(1.3)\qquad
\begin{aligned}
u,_i &\equiv [u(x_i+\Delta x_i/2) - u(x_i-\Delta x_i/2)]/\Delta x_i \\
u^i &\equiv [u(x_i+\Delta x_i/2) + u(x_i-\Delta x_i/2)]/2,
\end{aligned}
$$

so that $\partial_i u = \lim u,_i$ for $\Delta x_i \to 0$. Then corresponding to the product rule $\partial_i(uv) = u\partial_i v + v\partial_i u$ is the summation-by-parts formula

$$
(1.4)\qquad (uv),_i = u^i v,_i + v^i u,_i
$$

In order to help emphasize the natural correspondence between discrete and continuous results we shall let grad_h, div_h, curl_h denote the operators resulting by substituting central difference approximations in the corresponding differential operators. Then Gauss' theorem applies in the discrete form

$$
(1.5)\qquad \sum_{D_h} \mathrm{div}_h\, \underline{u}\, \Delta V = \sum_{\Gamma_h} (\underline{u}\cdot\underline{n})\Delta A.
$$

If r and s are 3 × 3 matrix valued functions we let

$$
(1.6)\qquad
\begin{aligned}
(r,s)_h &\equiv \sum_{D_h} \Big(\sum_{ij} r_{ij} s_{ij}\Big)\Delta V \\
\|r\|^2 &\equiv (r,r).
\end{aligned}
$$

We shall also find it convenient to employ the elementary tensor ε_{ijk} defined by

$$\begin{aligned}\varepsilon_{ijk} &= 1, && (i,j,k) = \text{even permutation of } (1,2,3),\\ &= -1, && (i,j,k) = \text{odd permutation of } (1,2,3),\\ &= 0, && \text{any equal indices;}\end{aligned}$$

thus

$$\operatorname{curl}_h \underline{u} = \Big(\sum_{ij} u_{j,i}\varepsilon_{ijk}\Big).$$

Using the notation (1.3) consider the finite difference equations

$$(1.7)\qquad \left.\begin{aligned} u_{j,i} - u_{i,j} &= \zeta_k\varepsilon_{ijk} && (\operatorname{curl}_h \underline{u} = \underline{\zeta})\\ \sum_i u_{i,i} &= \rho && (\operatorname{div}_h \underline{u} = \rho)\end{aligned}\right\} \quad \text{in } D_h$$

with

$$\underline{u}\cdot\underline{n} = g \qquad \text{in } \Gamma_h.$$

Take $s = s(\underline{u}) \equiv \operatorname{grad}_h \underline{u} \equiv (u_{i,j})$ and consider a choice of $r = r(v)$ such that summation-by-parts is possible in $(r(v),s(u))_h$: since

$$(1.8)\qquad \begin{aligned} r_{ii}u_{i,i} &= r_{ii}\Big(\rho - \sum_{j\neq i} u_{j,j}\Big),\\ r_{ij}u_{i,j} &= r_{ij}\big(u_{j,i} - \zeta_k\varepsilon_{ijk}\big), \quad j \neq i,\end{aligned}$$

the notation (1.3) suggests the choice $r = r(v)$ given by

$$r_{ii} = v_{ii}^{jk} \quad , \qquad i \neq j \neq k$$

(1.9)

$$r_{ij} = v_{ij}^{i} \quad , \qquad i \neq j \, .$$

Using (1.4) and (1.8) as well as a certain amount of formal manipulation, this leads to

(1.10)
$$\sum_{i,j} r_{ij}(v)s_{ij}(u) = \rho\rho' + \underline{\zeta}\cdot\underline{\zeta}' + \mathrm{div}_h\, \underline{q}$$

$$+ \sum_i u_i^i \sigma_i + \sum_i \Big(\sum_{j\neq i} v_{ji,j}\tau_{ij}\Big),$$

in which

$$\rho' = \sum_{i\neq j\neq k} v_{ii}^{jk},$$

$\underline{\zeta}' = (\zeta_1', \zeta_2', \zeta_3')$ with

$$\zeta'_k = \sum_{i\neq j\neq k} v_{ij}^{i}\varepsilon_{jik},$$

$\underline{q} = (q_1, q_2, q_3)$ with

(1.11)
$$q_i = v_{ij}u_j + v_{ik}u_k - u_i(v_{jj}^k + v_{kk}^j), \qquad i\neq j\neq k$$

while
$$\sigma_i = \sum_{i\neq j\neq k} (v_{jj,i}^k - v_{ji,j})$$

and

$$\tau_{ij} = u_i^i - u_i^j.$$

When

(1.12)
$$\sigma \equiv (\sigma_i) = 0, \qquad \tau_{ij} = 0,$$

in (1.10) there then results the summation identity

$$(1.13) \qquad \big(r(v),s(u)\big)_h = \sum_{D_h} (\rho\rho' + \underline{\zeta}\cdot\underline{\zeta}')\Delta V + \sum_{\Gamma_h} (\underline{q}\cdot\underline{n})\Delta A.$$

Note that the expression $(r(v),s(u))_h$ involves only averages or differences of v or u, i.e., only the values of these variables on the faces of the elementary cells $\{\pi\}$ which cover D. The same is true of the defining equations (1.7) as well as conditions (1.12)

2. A Variational Formulation

Consider the finite dimensional space H_h having the inner product $(r(v),s(u))_h$. In H_h the spaces $\Omega(v)$, $\Omega(u)$ defined by

$$(2.1) \qquad \begin{array}{llll} \Omega(v): & \underline{\zeta}' = 0,\ \underline{\sigma} = 0 & & \text{in } D_h \\ & v_{ij} = 0 & (j \neq i) & \text{on } \Gamma_h \\ \Omega(u): & \rho = 0,\ \tau_{ij} = 0 & & \text{in } D_h \\ & \underline{u}\cdot\underline{n} = 0 & & \text{on } \Gamma_h, \end{array}$$

are orthogonal, i.e., $\big(\Omega(v),\Omega(u)\big) = 0$. Suppose that the manifolds

$$(2.2) \qquad \begin{array}{llll} \Omega_0(v): & \sum_{i,j} v^i_{ij}\varepsilon_{jik} = \zeta_k,\ \underline{\sigma} = 0 & & \text{in } D_h \\ & v_{ij} = \partial_j g & (j \neq i) & \text{on } \Gamma_h \\ \Omega_0(u): & \mathrm{div}_h\ \underline{u} = \rho & & \text{in } D_h \\ & \tau_{ij} = 0 & & \\ & \underline{u}\cdot\underline{n} = g & & \text{on } \Gamma_h, \end{array}$$

have a common point of intersection (u^*,v^*) satisfying $r(v^*) = s(u^*)$. This point may be obtained as the solution of the following variational problems (c.f. [1]):

$$\text{(2.3)} \qquad \begin{aligned} &\text{I.} \quad \min_{v \,\varepsilon\, \Omega_0(v)} \| r(v) - s(u^*) \| = 0 \\ &\text{II.} \quad \min_{u \,\varepsilon\, \Omega_0(u)} \| r(v^*) - s(u) \| = 0. \end{aligned}$$

These variational problems are reciprocal in the sense that the admissibility conditions for one are the Euler equations for the other.

As a result, (1.13) yields

$$\text{(2.4)} \qquad \| \mathrm{grad}_h\, u^* \|^2 = \sum_{D_h} \left[(\mathrm{div}_h u^*)^2 + (\mathrm{curl}_h u^*)^2 \right] \Delta V + \sum_{\Gamma_h} (\underline{q}^* \cdot \underline{n}) \Delta A,$$

where, if $q^* = (q_1^*, q_2^*, q_3^*)$,

$$\text{(2.5)} \qquad q_i^* = (\partial_j g) u_j^* + (\partial_k g) u_k^* - g(v_{jj}^{*k} + v_{kk}^{*j}).$$

The common solution v^* and u^* of the variational problems (2.3) are thus related by $r(v^*) = s(u^*)$, i.e.,

$$\text{(2.6)} \qquad (v_{ii}^*)^{jk} = u_{i,i}^*, \qquad (v_{ij}^*)^i = u_{i,j}^*, \qquad i \neq j \neq k,$$

and satisfy equations (2.12). If $g = 0$ on Γ reference to (2.5) shows that $\underline{q}^* \cdot \underline{n} = 0$ also; for the homogeneous problem in which $\mathrm{div}_h\, \underline{u} = 0$, $\mathrm{curl}_h\, \underline{u} = 0$, and $g = 0$ (2.4) then implies $\mathrm{grad}_h\, \underline{u} = 0$ in D_h and it is follows that $\underline{u} \equiv 0$ in D_h. The difference equations (2.2) and (2.6) thus have a unique solution.

It is easy to verify that these equations are consistent with the differential equations (1.1) (the compatability conditions $\partial_i \partial_j u = \partial_j \partial_i u$ imply the consistency of the condition $\underline{\sigma} = 0$ in (2.2); the correspondence of (2.4) with (1.2) is also evident).

3. The Algebraic Problem

In the three-dimensional case the algebraic system expressed by (2.6) and (2.2) is overdetermined. This section will describe a finite difference scheme which results in a determined system of equations.

Suppose D_h is composed of N^3 cells and that Γ_h has $6N^2$ cell faces. There are then a total of $f = 3N^2(N+1)$ faces of cells $\{\pi\}$ which lie in D_h and Γ_h. The values of v and u in (2.6) and (2.2) are associated with the faces of these cells, hence there are a total of 9f variables v and 3f variables u to be determined. The number of admissibility conditions (2.2) for the manifold $\Omega_0(v)$ is $7N^3 + 12N^2$ while $\Omega_0(u)$ involves $7N^3 + 6N^2$ the additional $9N^3$ conditions (2.6) expressing $r(v) = s(u)$ thus lead to a total of $23N^3 + 18N^2$ conditions for the $(9+3)f$ variables.

In order to obtain a determined system of algebraic equations for the $3f = 9N^2(N+1)$ variables u we may add to the $7N^3 + 6N^2$ admissibility conditions for $\Omega_0(u)$ any additional $2N^3 + 3N^2$ admissibility conditions for $\Omega_0(v)$ since the latter also express the Euler conditionns for the variational problem for u. Specifically, we may consider the following: to the $9N^3 + 6N^2$ equations

$$
(3.1)\qquad
\begin{array}{rcll}
\mathrm{div}_h\, \underline{u} &=& 0 & \\
u_{3,2} - u_{2,3} &=& \zeta_1 & \text{in } D_h \\
u_{1,3} - u_{3,1} &=& \zeta_2 & \\
\underline{u}^i &=& \underline{u}^j \quad (i \neq j) & \\
\underline{u} \cdot \underline{n} &=& g & \text{on } \Gamma_h,
\end{array}
$$

impose the additional conditions

$$
(3.2)\qquad u_{2,1} - u_{1,2} = \zeta_3,
$$

in any $3N^2$ cells in D_h. The result is then a determined system of algebraic equations whose solution provides u^*. The variational formulation shows that equation (3.2) will also be satisfied in each of the N^3 cells of D_h.

The relationship of this result to the continuous problem may be interpreted as follows: the identity div curl $\underline{w} = 0$ which implies a linear relationship between the components of the vorticity $\underline{\zeta}$ = curl $\underline{w}$ is a consequence of the compatability conditions $\partial_i \partial_j w = \partial_j \partial_i w$. This dependency is only approximately expressed by the finite difference equations; here one of the components of $\mathrm{curl}_h\, \underline{w} = \underline{\zeta}$ may be given at $3N^2$ cells whereas the other two components are to be specified throughout the N^3 cells of D_h (3.1); then, necessarily, $\mathrm{curl}_h\, \underline{w} = \underline{\zeta}$ throughout D_h.

We shall not describe effective numerical procedures to solve (3.1) and (3.2) except to observe that the general SOR type scheme described by Kaczmarz [3] is applicable. This scheme was utilized in [2] to treat this problem in two-dimensions where, it is worth observing, a determined system of finite-difference equations is described by

$$
(3.3) \qquad \begin{aligned}
\mathrm{div}_h\, \underline{u} &= 0 \\
u_{2,1} - u_{1,2} &= \zeta_3 && \text{in } D_h \\
\underline{u}^i &= \underline{u}^j \qquad (i \neq j) \\
\underline{u}\cdot\underline{n} &= g && \text{on } \Gamma_h.
\end{aligned}
$$

Box-variables

The difference equations (3.1) and (3.2) (in two-dimensions, (3.3)) can be more economically solved by the use of box-variables described as follows: in a cell π let ω_i denote a face parallel to x_i = const. and let $u(\omega_i)$ indicate a value associated with the face ω_i which arises in the finite difference equations. Associate with the vertices of the cell π values $\underline{z}_i$, called box-variables, satisfying

$$
(3.4) \qquad u(\omega_i) = \underline{z}^{jk} \quad , \qquad i \neq j \neq k
$$

Then the conditions $\underline{u}^i = \underline{u}^j$ $(i \neq j)$ in (3.1) are satisfied identically and the remaining equations in (3.1) and (3.2) reduce in number to a total of $3N^2(N+3)$. The total number of variables introduced by (3.4) is $3(N+1)^3$ so that the components of $\underline{z}$ may be given arbitrarily at $(3N+1)$ vertices in order to solve (3.1) and (3.2) in terms of the box-variables $\underline{z}$. In contrast, in two dimensions the components of $\underline{z}$ may be given arbitrarily at one vertex point.

4. Convergence

For an arbitrary mesh-valued function $\underline{u}$ such that $\underline{u}\cdot\underline{n} = 0$ on Γ_h the identity (1.10) leads, by taking $r(v) = s(u)$, to

(4.1)

$$\|\mathrm{grad}_h\, \underline{u}\|^2 = \sum_{D_h} [(\mathrm{div}_h\, \underline{u})^2 + (\mathrm{curl}_h\, \underline{u})^2]\Delta V + \sum_{D_h} \sum_{i} (u_i^i \sigma_i + \sum_{j\neq i} v_{ji,j}\tau_{ij})\Delta V.$$

Let ε_h denote the difference between the solution $\underline{u}$ of the differential equation (1.1) and the solution $\underline{u}_h$ of the finite difference equations (3.1) and (3.2). Noting (1.11) and (2.6), then $\sigma(\underline{\varepsilon}_h) = 0(h^2)$, $\tau(\underline{\varepsilon}_h) = 0(h^2)$, while $\mathrm{curl}_h\, \underline{\varepsilon}_h = 0(h^2)$ and $\mathrm{div}\, \varepsilon_h = 0(h^2)$. Thus $\|\mathrm{grad}_h\, \underline{\varepsilon}_h\| = 0(h)$ and hence also $\|\underline{\varepsilon}_h\| = 0(h)$. As noted in the introduction, this may not be the strongest possible estimate; however it is sufficient to establish the convergence of the finite-difference scheme (3.1)-(3.2).

5. Concluding Remarks

The accurate solution of boundary value problems depends critically upon an accurate treatment of the boundary conditions. Because the finite difference scheme described above is based upon the use of rectangular subdomains it can lead to an inaccurate representation of data on curved boundaries. However, if simple finite difference analogue of the chain rule which has been described in Philips and Rose [5] is employed at boundaries to transform the difference equations from a rectangular cell a more effective means of treating nonrectangular domains can result.

Finally, Tanabe [6] has shown that the Kaczmarz algorithm can be applied to obtain the least squares solution of a system of equations. This permits a direct means of treating (3.1) when the vorticity equation (3.2) for ζ_3 is imposed throughout D_h. The treatment of (1.1) as described by (3.1) and (3.2) (or using the box variables (3.4)) should help clarify the relationship of the least squares problem to a fully determined algebraic system.

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